INFRARED SPECTRA OF MOLECULES AND MATERIALS OF ASTROPHYSICAL INTEREST

Grant NGR-41-002-003

Semi-Annual Progress Report

Report Number 1

December 1965

Office of Grants and Research Contracts
Office of Space Science and Applications
National Aeronautics and Space Administration
Washington, D. C. 20546

(Prepared under Grant NGR-41-002-003 by the University of South Carolina, Columbia, South Carolina 29208)

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Period Covered: 1 June 1965 to 30 November 1965

The infrared spectra of liquid, solid and gaseous tetradeuterated hydrazine have been measured from 250 to 4000 cm^{-1} using a Perkin-Elmer Model 521 Spectrophotometer. The spectrum of the gas phase was recorded using maximum pressure at room temperature with path lengths of 10 and 100 cm. The infrared of the liquid was recorded using a liquid cell with a 0.007 mm Teflon spacer and Irtran II windowns. A cold cell similar to that used by Wagner and Hornig[1] was used to record the infrared spectrum of the solid. Fine structure was resolved for three of the perpendicular fundamental bands of the assumed symmetric top. The Raman spectra of liquid hydrazine and tetradeuterated hydrazine have been recorded using a Cary Model-81 Raman Spectrophotometer and depolarization values measured using Polaroid cylinders.[2] A complete vibrational analysis based on band type, position, and depolarization values has been made which satisfies the product rule for both vibrational symmetry species a and b. The intensity of the 3189 cm^{-1} band of hydrazine has been studied as a function of temperature. Values of $\Delta H°$, $\Delta F°$, and $\Delta S°$ for H-bond formation in hydrazine are found to be -1750 cal/mole, 2060 cal/mole and -12.8eu respectively at 25°C.

Matrix Spectrum of N_2D_4

As a continuation of our studies on hydrazine-d_4 we have investigated the infrared spectrum of N_2D_4 in an argon matrix with mole ratios of 500 to 1 and 300 to 1 at 20°K. All spectra were recorded on a Perkin-Elmer Model-521 Spectrophotometer using a liquid hydrogen cryostat purchased from Air Products, Allentown, Pennsylvania. Bands were observed at 2770, 2733, 2505, 2445, 2427, 2349, 1197, 1191, 1136, 1039, 1033, 971, 965, 953, 936, 924, 248, 806, 771, 732, 693, 680, 655 and 285 cm^{-1}. The spectrum was much more complicated than expected and a satisfactory analysis of the

spectrum will require additional data at several more concentrations. Different sampling techniques may also have to be developed.

Matrix Spectrum of CH_3NH_2

We have initiated an infrared study of methyl amine in an argon matrix with a mole ratio of 300 to 1. Instrumental techniques were similar to those described in the previous paragraph. The following bands were observed: 3380, 3280, 3170, 2950, 2910, 2890, 2800, 1615, 1605, 1475, 1460, 1150, 1040, 980, 865 broad, 792, 425, 370 and 250 cm^{-1}. The N-H stretching vibrations are assigned to bands at 3380 and 3280 cm^{-1}. The C-H stretching vibrations are assigned to the bands at 2950, 2890 and 2800 cm^{-1}. The NH_2 deformation is assigned to the split band at 1615 and 1605 cm^{-1}. The three CH_3 deformations are assigned to the two bands at 1475 and 1460 cm^{-1} assuming the other CH_3 deformation to be degenerate with either the 1475 or 1460 cm^{-1} band. The two CH_3 wagging vibrations appear at 1150 cm^{-1} with a shoulder on the high frequency side of the band. The NH_2 wagging is unquestionably assigned to the 792 cm^{-1} band and the torsional vibration to the band at 250 cm^{-1}. The C-N stretching is assigned to the band at 1040 cm^{-1}. The NH_2 twisting remains to be assigned and the strong band at 865 cm^{-1} has not been assigned to a normal vibration. We do not wish to speculate on these assignments until we have recorded the infrared spectra of CD_3NH_2 and CH_3ND_2 in an argon matrix. These materials will shortly be on hand and the next phase of our research will be to record and analyze the spectra of CD_3NH_2 and CH_3ND_2.

Bibliography

1. E. L. Wagner and D. F. Hornig, J. Chem. Phys., 18, 296 (1950).

2. B. L. Crawford, Jr., and W. Horwitz, J. Chem. Phys., 15, 268 (1947).